S(e)MR

СИБИРСКИЕ ЭЛЕКТРОННЫЕ
МАТЕМАТИЧЕСКИЕ ИЗВЕСТИЯ
Siberian Electronic Mathematical Reports
http://semr.math.nsc.ru
ISSN 1813-3304

Vol. 21, No. 2, pp. **144–145** *(2024)*
https://doi.org/10.33048/semi.2024.21.???

УДК 519.61
MSC 15B33

AN EFFICIENT COMPLEX STRUCTURE-PRESERVING ALGORITHM FOR THE AUTONNE-TAKAGI DECOMPOSITION OF QUATERNION MATRICES

GANG WANG

Communicated by P.P. Petrov

Abstract: Given the importance of the Autonne-Takagi decomposition in fields such as quantum computing and signal processing and the research gap in this decomposition algorithm in quaternionic mechanics. This paper investigates the algorithm for computing the Autonne-Takagi decomposition of quaternion matrices, that is, special singular value decomposition algorithms for η-Hermitian quaternion matrices. Effective algorithms for rotation transformations of quaternion matrices are developed, including the realization function, imaginary function, and Householder function based on complex representation matrices of quaternion matrices. Furthermore, an efficient complex structure-preserving algorithm for the Autonne-Takagi decomposition of η-Hermitian quaternion matrices is established for the first time. Numerical experiments confirm the strong performance of the proposed algorithms, which are expected to enhance the research and application of the quaternion algebra in areas like quantum mechanics and signal processing.

Keywords: quaternion matrices, Autonne-Takagi decomposition, singular value decomposition, structure-preserving algorithm.

Wang, G., An efficient complex structure-preserving algorithm for the Autonne-Takagi decomposition of quaternion matrices.

The work is supported by the Russian Science Foundation (grant 23-71-30013) and the Chinese Government Scholarship (grant CSC.202008370340).

Received August, 30, 2024, Published.

1 Introduction

As scholars delve deeper into the research and development of quaternions, these algebraic structures are increasingly pivotal across various domains. Applications extend to fields such as quantum mechanics [1, 2], electromagnetics [3], computer vision [4], signal and color image processing [5, 6]. Despite the challenges posed by their non-commutative multiplication, which has somewhat constrained the advancement of their algebraic theories and algorithms, scholars remain enthusiastic about exploring their diverse applications. In particular, since efficient matrix decomposition algorithms can effectively improve the computational speed and effect of practical application problems, researchers have shown significant interest in investigating these intricate algorithms. Some known research results include LU decomposition [7, 8], QR decomposition [9, 10], eigen-decomposition [11, 12], Schur decomposition [13], SVD [14], GSVD [15, 16], etc.

Autonne-Takagi decomposition is a crucial tool for effectively addressing complex matrix decomposition problems in advanced fields such as quantum mechanics and signal processing. Its unique capabilities enhance computational efficiency and applicability in these demanding domains. In papers [17, 18], K. Fujikawa utilized the Autonne-Takagi decomposition to ensure that CP symmetry remains good in the presence of lepton number-violating neutrino mass terms, thus aligning with the classical Majorana condition for emergent Majorana fermions. S.M. Assad et al. exploited the Autonne-Takagi decomposition to eliminate correlations between conjugate quadratures in Gaussian quantum states and provided explicit expressions for these operations when such elimination was possible in [19]. In papers [20, 21], C.M. Caves and M. Houde et al. summarized several important matrix decompositions commonly used in quantum optics, namely Takagi/Autonne, Bloch-Messiah/Euler, polar decomposition, Iwasawa and Williamson decomposition. Given the pivotal role of the quaternion algebra across various fields, there is a pressing need for specialized matrix decomposition techniques that can handle the unique properties of quaternion matrices. Among these, the Autonne-Takagi decomposition stands out as a crucial tool. In papers [22, 23], C.C. Took and F. Zhang et al. proved the theoretical existence of the Autonne-Takagi decomposition in the quaternion algebra. However, while the theoretical foundations are established, there remains a significant gap in developing efficient algorithms for performing this decomposition in practical applications. Addressing this gap is essential for leveraging the Autonne-Takagi decomposition's full potential, particularly in complex scenarios where quaternion matrices are involved. Hence, research into efficient algorithms for the Autonne-Takagi decomposition is vital for advancing theoretical understanding and practical implementation in relevant fields.

The purpose of this paper is to advance the practical application of quaternion matrices through the development of efficient algorithms. Using

the complex representation matrix of quaternion matrices and our previous research and understanding for complex structure-preserving algorithms of quaternion matrices [24, 25, 26, 27], we aim to achieve the following goals:
Algorithm development: The paper introduces several effective algorithms for rotation transformations of quaternion matrices, including the quaternion realization function, quaternion imaginary function, and quaternion Householder function, etc. These algorithms enhance the manipulation and application of quaternion matrices in various contexts.
Autonne-Takagi decomposition: It establishes, for the first time, an efficient complex structure-preserving algorithm for the Autonne-Takagi decomposition of η-Hermitian quaternion matrices. This includes procedures that are also applicable to the unitary eigen-decomposition of Hermitian and skew-Hermitian quaternion matrices.

The structure of this paper is as follows: In Section 2, the definition and algebraic properties of quaternions are reviewed, and some symbolic and complex representation matrices are given. In Section 3, the theorem derivation and algorithm description for the Autonne-Takagi decomposition of quaternion matrices are given. In addition, the realization function, imaginary function and Householder function required by the algorithm are also included. In Section 4, two numerical examples are used to prove the effectiveness of the algorithms proposed in this paper.

2 Preliminaries

I. Quaternion algebra. Quaternions are an algebraic extension of the complex number system, proposed by W. R. Hamilton in 1843 [28], and have the following form

$$q = q_1 + q_2\mathrm{i} + q_3\mathrm{j} + q_4\mathrm{k} \in \mathbf{Q}, \tag{1}$$

where $q_1, q_2, q_3, q_4 \in \mathbf{R}$, $\{\mathrm{i}, \mathrm{j}, \mathrm{k}\}$ are the fundamental units. $\mathbf{Q}$ denotes the skew-field of quaternions. Specifically, the multiplication rules for the units in quaternions are given by

$$\begin{cases} \mathrm{i}^2 = -1, \quad \mathrm{j}^2 = -1, \quad \mathrm{k}^2 = -1, \\ \mathrm{ij} = -\mathrm{ji} = \mathrm{k}, \quad \mathrm{jk} = -\mathrm{kj} = \mathrm{i}, \quad \mathrm{ki} = -\mathrm{ik} = \mathrm{j}. \end{cases} \tag{2}$$

Given a quaternion $q = q_1 + q_2\mathrm{i} + q_3\mathrm{j} + q_4\mathrm{k} \in \mathbf{Q}$, $\overline{q} = q_1 - q_2\mathrm{i} - q_3\mathrm{j} - q_4\mathrm{k}$ is the conjugate of q, the norm of q is defined to be $|q| = \sqrt{|q\overline{q}|} = \sqrt{|q_1^2 + q_2^2 + q_3^2 + q_4^2|}$.

Lemma 1. [29] *Let $p, q \in \mathbf{Q}$. Then the following are equivalent:*
(1) p and q are similar, that is, there is a nonzero quaternion s such that $p = sqs^{-1}$;
(2) p and q are similar if and only if $\mathrm{Re}(p) = \mathrm{Re}(q)$ and $|\mathrm{Im}(p)| = |\mathrm{Im}(q)|$.

Some symbols of quaternion matrices are given in Table 1 below.

Symbols	Names	Descriptions
A		$A = A_1 + A_2\mathrm{i} + A_3\mathrm{j} + A_4\mathrm{k} \in \mathbf{Q}^{m\times n}$
$\overline{A}$	conjugate	$\overline{A} = A_1 - A_2\mathrm{i} - A_3\mathrm{j} - A_4\mathrm{k} \in \mathbf{Q}^{m\times n}$
A^T	transpose	$A^T = A_1^T + A_2^T\mathrm{i} + A_3^T\mathrm{j} + A_4^T\mathrm{k} \in \mathbf{Q}^{n\times m}$
A^H	conjugate transpose	$A^H = A_1^T - A_2^T\mathrm{i} - A_3^T\mathrm{j} - A_4^T\mathrm{k} \in \mathbf{Q}^{n\times m}$
A	Hermitian	$A = A^H \in \mathbf{Q}^{n\times n}$
A	skew-Hermitian	$A = -A^H \in \mathbf{Q}^{n\times n}$
A^η	$\eta-$ conjugate transpose $\eta \in \{\mathrm{i},\mathrm{j},\mathrm{k}\}$	$A^\mathrm{i} = A_1^T - A_2^T\mathrm{i} + A_3^T\mathrm{j} + A_4^T\mathrm{k} \in \mathbf{Q}^{n\times m}$ $A^\mathrm{j} = A_1^T + A_2^T\mathrm{i} - A_3^T\mathrm{j} + A_4^T\mathrm{k} \in \mathbf{Q}^{n\times m}$ $A^\mathrm{k} = A_1^T + A_2^T\mathrm{i} + A_3^T\mathrm{j} - A_4^T\mathrm{k} \in \mathbf{Q}^{n\times m}$
A	η-Hermitian	$A = A^\eta \in \mathbf{Q}^{n\times n}$
A	unitary	$AA^H = A^HA = I_n$
$\|A\|_F$	norm	$\|A\|_F = \sqrt{\|A_1\|_F^2 + \|A_2\|_F^2 + \|A_3\|_F^2 + \|A_4\|_F^2}$

Таблица 1. Symbol table of quaternion matrices.

II. Complex representation matrix of quaternion matrices. Given $A = A_1 + A_2\mathrm{i} + A_3\mathrm{j} + A_4\mathrm{k} = M_1 + \mathrm{k}M_2 \in \mathbf{Q}^{m\times n}$, its complex representation matrix A^σ has the following form,

$$A^\sigma = \begin{bmatrix} M_1 & -\overline{M}_2 \\ M_2 & \overline{M}_1 \end{bmatrix} \in \mathbf{C}^{2m\times 2n}, \tag{3}$$

and

$$A^\sigma = \begin{bmatrix} A_c^\sigma & Q_m^T\overline{A_c^\sigma} \end{bmatrix}, \qquad Q_m^T A^\sigma Q_n = \overline{A^\sigma}, \tag{4}$$

where $M_1 = A_1 + A_2\mathrm{i}, M_2 = A_4 + A_3\mathrm{i} \in \mathbf{C}^{m\times n}, A_c^\sigma = \begin{bmatrix} M_1 \\ M_2 \end{bmatrix}, Q_t = \begin{bmatrix} 0 & I_t \\ -I_t & 0 \end{bmatrix}$, I_t is an identity matrix, Q_t is a unitary matrix. With (3) and (4), it is easy to obtain the following results.

$$\begin{cases} (A+B)^\sigma = A^\sigma + B^\sigma, \quad (AC)^\sigma = A^\sigma C^\sigma, \quad (aA)^\sigma = aA^\sigma, \\ (A+B)_c^\sigma = A_c^\sigma + B_c^\sigma, \quad (AC)_c^\sigma = A^\sigma C_c^\sigma, \quad (aA)_c^\sigma = aA_c^\sigma, \end{cases} \tag{5}$$

where $A, B \in \mathbf{Q}^{m\times n}, C \in \mathbf{Q}^{n\times p}, a \in \mathbf{R}$. Complex representation matrices of quaternion matrices are the core of the structure-preserving optimization algorithm, and the conversion of operations between quaternion matrices into corresponding complex matrix operations by (5) will effectively reduce the computational complexity.

3 Autonne-Takagi decomposition of quaternion matrices

This section will use the special form conversion between quaternion matrices (Hermitian matrix, skew-Hermitian matrix and η-Hermitian matrix), Givens transformation, Householder transformation, and Imaginary function to establish the Autonne-Takagi decomposition algorithm of η-Hermitian quaternion matrices. At the same time, the matrix decomposition uses the complex representation matrix optimization process given by formulas (3) and (5), all of which are complex number operations that maintain the quaternion structure, that is, the complex structure-preserving algorithm of the Autonne-Takagi decomposition of η-Hermitian quaternion matrices is obtained.

Theorem 1. *Suppose that $A \in \mathbf{Q}^{n\times n}$ is a η-Hermitian quaternion matrix, i.e., $A = A^{\eta}, \eta = \{\mathrm{i}, \mathrm{j}, \mathrm{k}\}$. Then there exist a unitary matrix $U \in \mathbf{Q}^{n\times n}$ such that*

$$A = U\Sigma U^{\eta}, \tag{6}$$

in which $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \cdots, \sigma_n), \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0, \sigma_s$ is a singular value of A.

Proof. In the paper [23], the existence of the Autonne-Takagi decomposition of a η-Hermitian quaternion matrix has been briefly introduced, and the brief derivation can be described as the following formulas.

$$\begin{cases} A^H\eta = VDV^H, \quad D = \mathrm{diag}(\tau_1, \tau_2, \cdots, \tau_n), \quad \mathrm{Re}(\tau_s) = 0, \quad s = 1, 2, \cdots, n, \\ \quad A = \eta^H A^H \eta = -\eta(VDV^H) = -\eta(VP\Sigma\eta P^H V^H) = -\eta(VP\Sigma\eta P^H V^H) \\ \qquad = (\eta VP)\Sigma(\eta^H P^H V^H) = (\eta VP)\Sigma(\eta^H (\eta VP)^H \eta) = U\Sigma U^{\eta}, \end{cases} \tag{7}$$

where $A^H\eta$ is a skew-Hermitian quaternion matrix, and its unitary eigen-decomposition is $A^H\eta = VDV^H$; $D = P\Sigma\eta P^H$ is a unitary similarity transformation based on Theorem 2; $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \cdots, \sigma_n), \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0, \sigma_s$ is a singular value of A; $U = \eta VP$ is a unitary matrix. □

Theorem 2. *Given a pure imaginary quaternion $q = a_2\mathrm{i} + a_3\mathrm{j} + a_4\mathrm{k} \in \mathbf{Q}$. Then there exist three unit quaternions $s = \frac{p}{|p|} \in \mathbf{Q}$ such that*

$$s^H q s = |q|\eta = \begin{cases} |q|\mathrm{i}, \quad \textit{where } p = -a_3 + (a_2 - a_4 + |q|)\mathrm{i} + a_3\mathrm{j} + (a_2 + a_4 - |q|)\mathrm{k}, \\ |q|\mathrm{j}, \quad \textit{where } p = a_2 - a_3 + a_4 - |q| + (a_2 - a_3 + a_4 + |q|)\mathrm{i} + \\ \qquad\qquad (a_2 + a_3 - a_4 + |q|)\mathrm{j} + (a_2 + a_3 + a_4 - |q|)\mathrm{k}, \\ |q|\mathrm{k}, \quad \textit{where } p = -2a_3 + (-2a_4 + 2|q|)\mathrm{i} + (2a_2)\mathrm{k}. \end{cases} \tag{8}$$

Proof. By Lemma 1, it is easy to prove that q is similar to $|q|\mathrm{i}$, $|q|\mathrm{j}$, and $|q|\mathrm{k}$. In addition, the unitary similarity transformation number can be obtained and proved by direct verification. The following Algorithm 1 gives the numerical code of the Imaginary function. In addition, the function QCR() in the following algorithm is a complex representation function based on the formula (3) and will not be described separately. □

Algorithm 1: Imaginary function of a quaternion: Given a pure imaginary quaternion $q = s_1 + \mathrm{k}s_2 \in \mathbf{Q}$, compute its similarity transformation complex representation matrix P.

Function $P=$ PIJK(s_1, s_2)

  $a_2 = \mathrm{imag}(s_1); a_4 = \mathrm{real}(s_2); a_3 = \mathrm{imag}(s_2);$

  Case 1: the unitary complex representation matrix of i-similarity

    $b_1 = -a_3;\ b_2 = a_2 - a_4 + \sqrt{a_2^2 + a_3^2 + a_4^2}; b_3 = a_3;\ b_4 = a_2 + a_4 - \sqrt{a_2^2 + a_3^2 + a_4^2};$

    $P = \mathrm{QCR}(b_1 + b_2\mathrm{i}, b_4 + b_3\mathrm{i})/\mathrm{norm}([b_1, b_2, b_3, b_4]);$

  Case 2: the unitary complex representation matrix of j-similarity

    $c_1 = -a_3 + a_2 + a_4 - \sqrt{a_2^2 + a_3^2 + a_4^2};\ c_2 = a_2 - a_4 + \sqrt{a_2^2 + a_3^2 + a_4^2} - a_3;$

    $c_3 = a_3 + a_2 - a_4 + \sqrt{a_2^2 + a_3^2 + a_4^2};\quad c_4 = a_2 + a_4 - \sqrt{a_2^2 + a_3^2 + a_4^2} + a_3;$

    $P = \mathrm{QCR}(c_1 + c_2\mathrm{i}, c_4 + c_3\mathrm{i})/\mathrm{norm}([c_1, c_2, c_3, c_4]);$

  Case 3: the unitary complex representation matrix of k-similarity

    $d_1 = -2a_3;\ d_2 = -2a_4 + 2\sqrt{a_2^2 + a_3^2 + a_4^2};\ d_3 = 0;\ d_4 = 2a_2;$

    $P = \mathrm{QCR}(d_1 + d_2\mathrm{i}, d_4 + d_3\mathrm{i})/\mathrm{norm}([d_1, d_2, d_3, d_4]);$

End

Based on Theorem 1 and its proof, the Autonne-Takagi decomposition of a η-Hermitian quaternion matrix A can be simply described as the following transformation process:

(1) η-Hermitian quaternion matrix $A \longrightarrow$ skew-Hermitian quaternion matrix B, i.e.,

$$A_c^\sigma = \begin{bmatrix} M_1 \\ M_2 \end{bmatrix} \xrightarrow{A^H\eta} \underset{A = A^{\mathrm{i}}}{\underset{\uparrow}{B_c^\sigma = \begin{bmatrix} M_1^H\mathrm{i} \\ -M_2^T\mathrm{i} \end{bmatrix}}} \text{ or } \underset{A = A^{\mathrm{j}}}{\underset{\uparrow}{B_c^\sigma = \begin{bmatrix} M_2^H\mathrm{i} \\ M_1^T\mathrm{i} \end{bmatrix}}} \text{ or } \underset{A = A^{\mathrm{k}}}{\underset{\uparrow}{B_c^\sigma = \begin{bmatrix} M_2^H \\ M_1^T \end{bmatrix}}}$$

where $A = M_1 + \mathrm{k}M_2 \in \mathbf{Q}^{n\times n}, M_1, M_2 \in \mathbf{C}^{n\times n}$.

(2) skew-Hermitian quaternion matrix $B \longrightarrow$ Hermitian quaternion matrix C, i.e.,

$$B_c^\sigma = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} \xrightarrow{C=B^H B} C_c^\sigma = \begin{bmatrix} B_1 & -\overline{B_2} \\ B_2 & \overline{B_1} \end{bmatrix} \begin{bmatrix} B_1^H \\ -B_2^T \end{bmatrix}$$

where $B = B_1 + \mathrm{k}B_2 \in \mathbf{Q}^{n\times n}, B_1, B_2 \in \mathbf{C}^{n\times n}$.

(3) Hermitian quaternion matrix $C \longrightarrow$ Real tridiagonal diagonal matrix T, this process is divided into two steps, respectively, using the quaternion Householder function to transform the matrix B into a complex tridiagonal matrix T_1 and then the quaternion realization function to transform the matrix T_1 into a real tridiagonal matrix T, i.e.,

$$B = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix} \xrightarrow[\times H_1^H]{H_1\times} \begin{bmatrix} \times & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \end{bmatrix} \xrightarrow[\times H_2^H]{H_2\times} \cdots \xrightarrow[\times H_{n-2}^H]{H_{n-2}\times} \begin{bmatrix} \times & \times & 0 & 0 & 0 \\ \times & \times & \times & 0 & 0 \\ 0 & \times & \times & \times & 0 \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix} = T_1$$

where H_t is a quaternion Householder transformation matrix. At this point, the main diagonal elements of the matrix T_1 are all real numbers, and the upper and lower diagonal elements are mutually conjugate quaternions. This is converted into a tridiagonal matrix by sequentially multiplying H_t and H_t^H to the left and right of B, respectively. The quaternion Householder transformation matrix is obtained by the following Lemma 2 and Algorithm 2.

Lemma 2. [30] *Suppose that* $x, y \in \mathbf{Q}^n, x \neq y$. *There exists a unit vector* $u = \frac{y-x}{\|y-x\|_2} \in \mathbf{Q}^n$ *such that* $Hy = (1-2uu^H)y = x$, *if and only if* $\|x\|_2 = \|y\|_2$ *and* $y^H x = x^H y$. *In particular, if* $y \in \mathbf{Q}^n$ *is not a multiple of* e_1, *which is the first column of unit matrix* I_n, *then the choice* $x = \alpha e_1$, *in which*

$$\alpha = \begin{cases} -\frac{y_1}{|y_1|}\|y\|_2, & y_1 \neq 0, \\ -\|y\|_2, & \text{otherwise}, \end{cases} \tag{9}$$

givens a reflection that maps y *to* αe_1. *The following Algorithm 2 gives the numerical code of the quaternion Householder function, and its corresponding Householder transformation matrix is* $H = I_n - \beta v v'$.

Algorithm 2: Householder function of a quaternion vector: Given a quaternion vector $x = x_1 + \mathrm{k}x_2 \in \mathbf{Q}^n$, compute its Householder vector $v = v_1 + \mathrm{k}v_2 \in \mathbf{Q}^n$ and the scalar $\beta \in \mathbf{R}$.

```
Function [v1, v2, β]= HouseholderQ(x1, x2)
    m = length(x1); v(1 : m, 1 : 2) = [x1, x2]; d = norm([x1; x2]); xx = norm([x1(1), x2(1)]);
    if xx == 0 then
        α = d * [1; 0];
    else
        α = −(d/xx) * ([x1(1), x2(1)]);
    end
    v(1, 1 : 2) = v(1, 1 : 2) − α;
    v1 = v(:, 1); v2 = v(:, 2); β = 1/(d * (d + xx));
End
```

$$T_1 = \begin{bmatrix} \times & \bar{*} & & & & \\ * & \times & \bar{*} & & & \\ & * & \times & \bar{*} & & \\ & & \ddots & \ddots & \ddots & \\ & & & * & \times & \bar{*} \\ & & & & * & \times \end{bmatrix} \xrightarrow[\times S_1^H]{S_1 \times} \begin{bmatrix} \times & \star & & & & \\ \star & \times & \bar{*} & & & \\ & * & \times & \bar{*} & & \\ & & \ddots & \ddots & \ddots & \\ & & & * & \times & \bar{*} \\ & & & & * & \times \end{bmatrix} \xrightarrow[\times S_2^H]{S_2 \times} \cdots \xrightarrow[\times S_{n-2}^H]{S_{n-2} \times} \begin{bmatrix} \times & \star & & & & \\ \star & \times & \star & & & \\ & \star & \times & \star & & \\ & & \ddots & \ddots & \ddots & \\ & & & \star & \times & \star \\ & & & & \star & \times \end{bmatrix} = T$$

where S_t is a quaternion rotation realization matrix. At this point, the main diagonal elements, the upper and lower diagonal elements of the matrix T are all real numbers. This is converted into a tridiagonal matrix by sequentially multiplying S_t and S_t^H to the left and right of T_1, respectively. The quaternion rotation realization matrix is obtained by the following Lemma 3 and Algorithm 3.

Lemma 3. *Suppose that* $q = s_1 + \mathrm{k}s_2 \in \mathbf{Q}, s_1, s_2 \in \mathbf{C}, |q| \neq 0$. *There exists a generalized Givens rotation matrix*

$$S = \begin{bmatrix} \cos\alpha_1 + \cos\alpha_2 \mathrm{i} & -\cos\alpha_4 + \cos\alpha_3 \mathrm{i} \\ \cos\alpha_4 + \cos\alpha_3 \mathrm{i} & \cos\alpha_1 - \cos\alpha_2 \mathrm{i} \end{bmatrix} \in C^{2\times 2} \tag{10}$$

such that $S^H q^\sigma = q^\sigma S^H = |q|I_2$, *that is, the purpose is to convert a quaternion into a real number by rotation. The following Algorithm 3 gives the numerical code of the realization function of the quaternion.*

Algorithm 3: Realization function of a quaternion: Given a quaternion $q = s_1 + \mathrm{k}s_2 \in \mathbf{Q}$, compute its realized rotation complex representation S.

Function $S=$ RFQ(s_1, s_2)
  if $[s_1, s_2] == 0$ **then**
    $S = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$;
  else
    $S = \begin{bmatrix} s_1 & -\bar{s}_2 \\ s_2 & \bar{s}_1 \end{bmatrix} / \sqrt{s_1\bar{s}_1 + s_2\bar{s}_2}$;
  end
End

(4) Real tridiagonal diagonal matrix $T \longrightarrow$ Real diagonal matrix D, i.e., the unitary eigen-decomposition of the real matrix $T = WDW^H$, where the diagonal elements of D are eigenvalues of T, the column vectors of W are the eigenvectors of T.

In summary, the complex structure-preserving algorithm of the Autonne-Takagi decomposition of quaternion matrices can be obtained as follows. Algorithm 4 is constructed as an example of the Autonne-Takagi decomposition of i-Hermitian quaternion matrices. The other two cases (j-Hermitian and k-Hermitian) can be done by slightly adjusting the first two sentences of the procedure according to step (1).

4 Numerical examples and analysis

Example 1. Given an i-Hermitian quaternion matrix $A \in \mathbf{Q}^{m\times n}$, where

$$A = \begin{bmatrix} 2 & 8 & 8 \\ 8 & 4 & 5 \\ 8 & 5 & 2 \end{bmatrix} + \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}\mathrm{i} + \begin{bmatrix} 4 & 2 & 6 \\ 2 & 10 & 4 \\ 6 & 4 & 8 \end{bmatrix}\mathrm{j} + \begin{bmatrix} 8 & 8 & 5 \\ 8 & 2 & 3 \\ 5 & 3 & 8 \end{bmatrix}\mathrm{k},$$

compute the Autonne-Takagi decomposition of A. By the Algorithm 4, we can get the results as follows:

$$\Sigma = \begin{bmatrix} 28.8102 & & \\ & 9.3634 & \\ & & 5.8566 \end{bmatrix},$$

$$U = \begin{bmatrix} 0.4592 & -0.0758 & -0.0002 \\ 0.3960 & 0.1982 & -0.2134 \\ 0.3924 & -0.2225 & 0.1106 \end{bmatrix} + \begin{bmatrix} -0.2677 & 0.1368 & -0.2556 \\ -0.3225 & -0.3259 & 0.0786 \\ -0.2912 & 0.2314 & 0.1697 \end{bmatrix}\mathrm{i}$$
$$+ \begin{bmatrix} -0.0787 & -0.5907 & -0.3417 \\ 0.0808 & 0.4309 & -0.3824 \\ 0.0996 & 0.2365 & 0.6352 \end{bmatrix}\mathrm{j} + \begin{bmatrix} 0.2677 & -0.1368 & 0.2556 \\ 0.2116 & 0.2235 & -0.3299 \\ 0.2807 & -0.2602 & -0.0369 \end{bmatrix}\mathrm{k},$$

where Σ and U satisfies $A = U\Sigma U^{\mathrm{i}}$, $\frac{\|A-U\Sigma U^{\mathrm{i}}\|_F}{\|A\|_F} = 1.3978 \times 10^{-15}$.

Example 2. Given η-Hermitian quaternion matrices $A = A_1 + A_2\mathrm{i} + A_3\mathrm{jk} + A_4\mathrm{k} \in \mathbf{Q}^{m\times n}$, where

$$m = 25, 50, \cdots, 500; \quad n = 25, 50, \cdots, 500;$$

$$B_1 = \mathrm{rand}(m, n);\ B_2 = \mathrm{rand}(m, n);\ B_3 = \mathrm{rand}(m, n);\ B_4 = \mathrm{rand}(m, n);$$

$$A = \begin{cases} (B_1^H + B_1) + (B_2^H - B_2)\mathrm{i} + (B_3^H + B_3)\mathrm{j} + (B_4^H + B_4)\mathrm{k}, & \text{if } \eta = \mathrm{i}; \\ (B_1^H + B_1) + (B_3^H + B_3)\mathrm{i} + (B_2^H - B_2)\mathrm{j} + (B_4^H + B_4)\mathrm{k}, & \text{if } \eta = \mathrm{j}; \\ (B_1^H + B_1) + (B_3^H + B_3)\mathrm{i} + (B_4^H + B_4)\mathrm{j} + (B_2^H - B_2)\mathrm{k}, & \text{if } \eta = \mathrm{k}. \end{cases}$$

Compute the CPU times and relative errors $\frac{\|A-U\Sigma U^{\eta}\|_F}{\|A\|_F}$ of A.

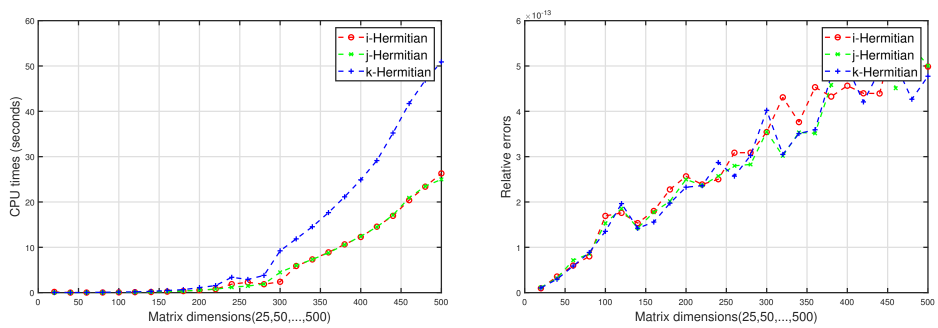

FIG. 1. CPU times and computation errors of Algorithm 4.

The left figure of Fig.1 shows the CPU times of the Autonne-Takagi decomposition for random $25, 50, \cdots, 500$-order i-Hermitian quaternion matrices, j-Hermitian quaternion matrices, and k-Hermitian quaternion matrices, which can all be decomposed in less than a minute. The speed of k-Hermitian matrix decomposition is slightly slower than the other two, which may be caused by different forms of matrix conversion at the beginning of the process. The right figure of Fig.1 shows the relative errors $\frac{\|A-U\Sigma U^{\eta}\|_F}{\|A\|_F}$ of the corresponding Autonne-Takagi decompositions. It is easy to see that the Algorithm 4 has a high accuracy rate.

5 Conclusions

In this paper, by using the complex representation matrix of quaternion matrices , the following main results are studied and obtained.

(1) Some effective algorithms for quaternion matrix rotation transformation are presented, including the quaternion realization function, quaternion imaginary function, quaternion Householder function, etc.

(2) An efficient complex structure-preserving algorithm for the Autonne-Takagi decomposition of η-Hermitian quaternion matrices is established for

the first time. In addition, some procedures involved in the algorithm are also valid for the unitary eigen-decomposition of Hermitian quaternion matrices and the unitary eigen-decomposition of skew-Hermitian quaternion matrices.

Finally, numerical experiments demonstrate the good performance of the proposed algorithms, which will surely promote the research and development of this 4D algebra in fields such as quantum mechanics and signal processing.

Algorithm 4: Autonne-Takagi decomposition function of a η-Hermitian quaternion matrix: Given a η-Hermitian matrix $A = M_1 + \mathrm{k}M_2 \in \mathbf{Q}^{n\times n}$, compute its Autonne-Takagi decomposition matrices $U = U_1 + \mathrm{k}U_2 \in \mathbf{Q}^{n\times n}$ and $S \in \mathbf{R}^{n\times n}$ such that $A = USU^{\eta}$. (Take i-Hermitian as an example)

```
Function [U1, U2, S] = ATDQ(M1, M2)
    [m, n] = size(M1);  B1 = M1' * i; B2 = -M2.' * i;  C = QCR(B1, B2) * [B1'; -B2.'];
    C1 = C(1 : n, :);  C2 = C(n + 1 : 2n, :);  T = [C1; C2];  V = [eye(m, m); zeros(m, m)];
    for s = 1 : n - 2 do
        if norm(T([s + 1 : n, n + s + 1 : 2n], s)) > 0 then
            [v1, v2, β] = HouseholderQ(T(s + 1 : n, s), T(n + s + 1 : 2n, s));
            H = β * QCR(v1, v2) * QCR(v1, v2)';
            T([s + 1 : n, n + s + 1 : 2n], s : n) = T([s + 1 : n, n + s + 1 : 2n], s :
              n) - H * T([s + 1 : n, n + s + 1 : 2n], s : n);
            V(:, s + 1 : n) = V(:, s + 1 : n) - QCR(V(1 : n, s + 1 : n), V(n + 1 : 2n, s + 1 :
              n)) * H(:, 1 : n - s);
            W = H';
            T(:, s + 1 : n) = T(:, s + 1 : n) - QCR(T(1 : n, s + 1 : n), T(n + 1 : 2n, s + 1 :
              n)) * W(:, 1 : n - s);
        end
    end
    for s = 1 : n - 2 do
        if norm([T(s + 1, s), T(n + s + 1, s)]) > 0 then
            G = RFQ(T(s + 1, s), T(n + s + 1, s));
            T([s + 1, n + s + 1], s : s + 2) = G' * T([s + 1, n + s + 1], s : s + 2);
            V(:, s + 1) = QCR(V(1 : n, s + 1), V(n + 1 : 2 * n, s + 1)) * G(:, 1);
            T(:, s + 1) = QCR(T(1 : n, s + 1), T(n + 1 : 2 * n, s + 1)) * G(:, 1);
        end
    end
    c = norm(T([n, 2n], n - 1));
    if c > 0 then
        V(:, n) = QCR(V(1 : n, n), V(n + 1 : 2n, n)) * [T(n, n - 1)/c; T(2n, n - 1)/c];
        T([n, 2n], n - 1) = [c; 0];    T([n - 1, 2n - 1], n) = [c; 0];
    end
    [VV, D] = schur(T(1 : n, :));    [PD, ind] = sort(diag(D), 'descend');
    VV = VV(:, ind);  D = diag(PD);  V = V * VV;
    WW = QCR(V(1 : n, :), V(n + 1 : 2n, :))' * QCR(B1, B2) * V;
    D1 = WW(1 : n, :);  D2 = WW(n + 1 : 2n, :);
    for t = 1 : n do
        d = norm([D1(t, t), D2(t, t)]);
        if d > 0 then
            P = PIJK(D1(t, t), D2(t, t));
            V(:, t) = QCR(V(1 : n, t), V(n + 1 : 2n, t)) * P(:, 1);
            s(t) = d;
        end
    end
    U1 = i * V(1 : n, :);  U2 = -i * V(n + 1 : 2n, :);  S = diag(s);
End
```

References

[1] S. Adler, *Quaternionic quantum mechanics and quantum fields*, Oxford University Press, New York, 1995.

[2] G. Wang, T. Jiang, V.I. Vasil'ev, Z. Guo, *On singular value decomposition for split quaternion matrices and applications in split quaternionic mechanics*, Journal of Computational and Applied Mathematics, **436** (2024), 115447.

[3] G. Wang, T. Jiang, V.I. Vasil'ev, Z. Guo, *An efficient method for Maxwell's equations with a discrete double-curl operator in split quaternionic electromagnetics*, The European Physical Journal Plus, **341** (2023), 138.

[4] X. Zhu, Y. Xu, H. Xu, C. Chen, *Quaternion convolutional neural networks*, Proceedings of the European conference on computer vision (ECCV), (2018), 631–647.

[5] N.L. Bihan, J. Mars, *Singular value decomposition of quaternion matrices: a new tool for vector-sensor signal processing*, Signal processing, **84**:7 (2004), 1177–1199.

[6] Y. Chen, X. Xiao, Y. Zhou, *Low-rank quaternion approximation for color image processing*, IEEE Transactions on Image Processing, **29** (2019), 1426–1439.

[7] M. Wang, W. Ma, *A structure-preserving method for the quaternion LU decomposition in quaternionic quantum theory*, Computer Physics Communications, **184**:9 (2013), 2182–2186.

[8] Y. Li, M. Wei, F. Zhang, J. Zhao, *A real structure-preserving method for the quaternion LU decomposition, revisited*, Calcolo, **54** (2017), 1553–1563.

[9] F. Zhang, J. Zhao, *A real structure-preserving algorithm based on the quaternion QR decomposition for the quaternion equality constrained least squares problem*, Numerical Algorithms, **91**:4 (2022), 1815–1827.

[10] Z. Guo, *A blind color watermarking technique based on quaternion complex structure-preserving QR decomposition*, Eurasian Journal of Mathematical and Computer Applications, **12**:1 (2024), 57–69.

[11] T. Jiang, Z. Guo, D. Zhang, V.I. Vasil'ev, *A fast algorithm for the Schrödinger equation in quaternionic quantum mechanics*, Applied Mathematics Letters, **150** (2024), 108975.

[12] T. Jiang, G. Wang, Z. Guo, D. Zhang, *Algebraic algorithms for a class of Schrödinger equations in split quaternionic mechanics*, Mathematical Methods in the Applied Sciences, **47**:7 (2024), 6205–6215.

[13] Z. Jia, M. Wei, M. Zhao, Y. Chen, *A new real structure-preserving quaternion QR algorithm*, Journal of Computational and Applied Mathematics, **343** (2018), 26–48.

[14] M. Zhang, W. Ding, Y. Li, J. Sun, Z. Liu, *Color image watermarking based on a fast structure-preserving algorithm of quaternion singular value decomposition*, Signal Processing, **208** (2023), 108971.

[15] T. Jiang, Z. Zhang, Z. Jiang, *A new algebraic technique for quaternion constrained least squares problems*, Advances in Applied Clifford Algebras, **28** (2018), 1–10.

[16] Z. Hu, S. Ling, Z. Jia, *Structure-preserving joint Lanczos bidiagonalization with thick-restart for the partial quaternion GSVD*, Numerical Algorithms, (2024), 1–22.

[17] K. Fujikawa, *Generalized Pauli–Gursey transformation and Majorana neutrinos*, Physics Letters B, **789** (2019), 76–81.

[18] K. Fujikawa, *Parity and CP operations for Majorana neutrinos*, Physical Review D, **102**:10 (2020), 105001.

[19] S.M. Assad, M. Gu, X. Li, P. Lam, *Decoupling cross-quadrature correlations using passive operations*, Physical Review A, **102**:2 (2020), 022615.

[20] C.M. Caves, *Polar decomposition, singular-value decomposition, and Autonne-Takagi factorization*, Quantum Information Lecture Notes, 2017.

[21] M. Houde, W. McCutcheon, N. Quesada, *Matrix decompositions in quantum optics: Takagi/Autonne, Bloch-Messiah/Euler, Iwasawa, and Williamson*, Canadian Journal of Physics, 2024.

[22] C.C. Took, D.P. Mandic, F.Z. Zhang, *On the unitary diagonalisation of a special class of quaternion matrices*, Applied Mathematics Letters, **24**:11 (2011), 1806–1809.
[23] R.A. Horn, F.Z. Zhang, *A generalization of the complex Autonne–Takagi factorization to quaternion matrices*, Linear and Multilinear Algebra, **60**:11-12 (2012), 1239–1244.
[24] G. Wang, D. Zhang, V.I. Vasil'ev, T. Jiang, *A complex structure-preserving algorithm for the full rank decomposition of quaternion matrices and its applications*, Numerical Algorithms, **91** (2022), 1461–1481.
[25] G. Wang, *A real structure-preserving algorithm for the low-rank decomposition of pure imaginary quaternion matrices and its applications in signal processing*, Eurasian Journal of Mathematical and Computer Applications, **11**:4 (2023), 117–129.
[26] Z. Guo, T. Jiang, V.I. Vasil'ev, G. Wang, *Complex structure-preserving method for Schrödinger equations in quaternionic quantum mechanics*, Numerical Algorithms, **97** (2024), 271–287.
[27] D. Zhang, T. Jiang, C. Jiang, G. Wang, *A complex structure-preserving algorithm for computing the singular value decomposition of a quaternion matrix and its applications*, Numerical Algorithms, **95** (2024), 267–283.
[28] W.R. Hamilton, *On a new species of imaginary quantities, connected with the theory of quaternions*, Proceedings of the Royal Irish Academy, **2** (1840), 424–434.
[29] F.Z. Zhang, *Quaternions and matrices of quaternions*, Linear Algebra and Its Applications, **251** (1997), 21–57.
[30] M. Wei, Y. Li, F. Zhang, J. Zhao, *Quaternion matrix computations*, Nova Science Publishers, 2018.

Gang Wang
Institute of Mathematics and Information Science,
North-Eastern Federal University,
677000, Yakutsk, Russia

School of Mathematical Sciences,
Qufu Normal University,
273165, Shandong, P. R. China
Email address: wang_gang93@163.com